

Excited state entanglement in homogeneous fermionic chains.

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We study the Rényi entanglement entropy of an interval in a periodic fermionic chain for a general eigenstate of a free, translational invariant Hamiltonian. In order to analytically compute the entropy we use two technical tools. The first one is used to reduce logarithmically the complexity of the problem and the second one to compute the Rényi entropy of the chosen subsystem. We introduce new strategies to perform the computations, derive new expressions for the entropy of these general states and show the perfect agreement of the analytical computations and the numerical outcome. Finally we discuss the physical interpretation of our results and generalise them to compute the entanglement entropy for a fragment of a fermionic ladder.

I. INTRODUCTION

In the last two decades, a great effort has been made to quantify the degree of entanglement between two quantum systems. Indeed, there are different ways to measure quantum correlations [1, 2]. One appropriate magnitude which can be used for this pur-

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pose is the von Neumann entropy of the reduced state. Suppose we have a bipartite system (i.e. it consists of two subsystems X and Y) so the Hilbert space can be expressed as the tensor product $\mathcal{H} = \mathcal{H}_X \otimes \mathcal{H}_Y$ of the Hilbert space of each subsystem. Let ρ be the density matrix which describes the state of the system. The von Neumann entropy of the subsystem X is defined as

$$S_1(X) = -\text{Tr}(\rho_X \log \rho_X) \quad (1)$$

where ρ_X is the reduced density matrix of X , i. e. $\rho_X = \text{Tr}_Y(\rho)$ with Tr_Y denoting the partial trace to the subsystem Y . $S_1(X)$ can be interpreted as a measure of the information which X and Y share. By definition $S_1(X) \geq 0$, and the zero value is attained when the state is separable into the tensor product. Besides, if the total system is in a pure state $|\psi\rangle$, i. e. $\rho = |\psi\rangle\langle\psi|$, then $S_1(Y) = S_1(X)$. A generalisation of the von Neumann entropy is the so-called Rényi entropy defined for any $\alpha > 1$ as

$$S_\alpha(X) = \frac{1}{1-\alpha} \log \text{Tr}(\rho_X^\alpha). \quad (2)$$

In fact when we take the limit $\alpha \rightarrow 1$ we recover the expression (1). Both entropies share the same general properties so that the Rényi entropy of the reduced density matrix can also be employed to measure the entanglement.

The von Neumann entropy has been specially studied in extended quantum systems because it is a very suitable quantity to analyse their universal properties in the neighbourhood of quantum critical points [3]. In this respect, a well-known result is the von Neumann entropy when X is a single interval of length L in a fermionic, unidimensional chain of N sites, in the ground state of a conformal critical Hamiltonian, with periodic boundary conditions. In this case one has [4–6]

$$S_1(X) = \frac{c}{3} \log \left(\frac{N}{\pi} \sin \frac{\pi L}{N} \right) + C_1 \simeq \frac{c}{3} \log L + C_1, \quad N \rightarrow \infty,$$

or for the Rényi entropy

$$S_\alpha(X) = \frac{1+\alpha}{\alpha} \frac{c}{6} \log \left(\frac{N}{\pi} \sin \frac{\pi L}{N} \right) + C_\alpha \simeq \frac{1+\alpha}{\alpha} \frac{c}{6} \log L + C_\alpha, \quad N \rightarrow \infty. \quad (3)$$

Here c is the central charge of the underlying conformal field theory and C_α a non universal constant that will be computed later. However, less attention has been paid to the case when the system is in an excited state which can strongly change the behaviour of the

entropy [7–12]. In this paper we study the Rényi entropy for certain particular states, not only the ground state, in a unidimensional fermionic chain.

In order to carry out the computation we shall make use of two technical tools. The first one is based on the work of Peschel [13] and allows to reduce the dependence of the complexity of the problem on the size of the system from 2^L to L . Instead of studying the reduced density matrix it is enough to consider the two-point correlation matrix. The second tool can be applied when the correlation matrix has the Toeplitz form, as it is in our case. Then we can find the behaviour of the Rényi entropy in the thermodynamic limit using the Fisher-Hartwig conjecture (or rather theorem, as it has been proven in our case [14]).

The paper extends the works of Jin and Korepin [15] and Alba, Fagotti and Calabrese [7] which employ the previously mentioned techniques to compute the entanglement in excited states (see also refs. [9, 16–18] for other approaches to the subject). We also generalise these techniques to derive the Rényi entropy for a piece of a fermionic ladder.

The paper is organised as follows. In the next section we formulate precisely the problem and fix the notation. In section III we discuss the connection between the reduced density matrix and the two-point correlation matrix for cases in which the Wick decomposition applies. In section IV we study the conditions under which the correlation matrix is of the Toeplitz type and the Fisher-Hartwig conjecture holds. Section V is devoted to the analytic evaluation of the Rényi entropy for our general case, while some particular examples and its comparison with the numerical results are discussed in section VI. In section VII we address the physical interpretation of our results and their connection with fermionic chains and ladders. We also compute the entanglement entropy for a fragment of a ladder. Finally, in section VIII we present a few conclusions and comments.

II. STATEMENT OF THE PROBLEM

Our system consists in a chain of N identical, spinless fermions with a_n and a_n^\dagger , $n = 1, \dots, N$ representing respectively the annihilation and creation operator for the site n . The only non vanishing anticommutation relations are

$$\{a_n, a_m^\dagger\} = \delta_{nm}.$$

We shall consider states that can be written as a Slater determinant, i.e.

$$|\Psi_{\mathcal{K}}\rangle = \prod_{k \in \mathcal{K}} b_k^\dagger |0\rangle \quad (4)$$

where $|0\rangle$ represents the vacuum in the Fock space,

$$b_k^\dagger = \sum_{n=1}^N \varphi_k^*(n) a_n^\dagger, \quad k = 1 - N/2, \dots, N/2,$$

is a basis for the creation operators such that b_k and b_k^\dagger satisfy canonical anticommutation relations and $\mathcal{K} \subset \{1 - N/2, \dots, N/2\}$ is the subset of excited modes in $|\Psi_{\mathcal{K}}\rangle$.

In actual applications, we shall consider a free, translational invariant Hamiltonian, like that of the Tight Binding Model with periodic boundary conditions

$$H = -T \sum_{n=1}^N a_n^\dagger (a_{n-1} + a_{n+1}), \quad (5)$$

and the state $|\Psi_{\mathcal{K}}\rangle$ is going to be an eigenstate of the Hamiltonian. For the moment, however, we will keep the discussion completely general without making any particular assumptions on the operators b_k .

Now we decompose the chain into two subsets $X = \{1, \dots, L\}$ and $Y = \{L+1, \dots, N\}$. Adapted to this decomposition we can factor out the Hilbert space $\mathcal{H} = \mathcal{H}_X \otimes \mathcal{H}_Y$. The goal is to study the entanglement between the two subsystems.

In order to do that we introduce the reduced density matrix $\rho_X = \text{Tr}_Y(|\Psi_{\mathcal{K}}\rangle\langle\Psi_{\mathcal{K}}|)$, that in general does not correspond to a pure state, and compute its Rényi entropy. As it was discussed before the entropy of the subsystem X coincides with that of the subsystem Y and provides a measurement for the entanglement between both subsystems.

Once we have obtained the reduced density matrix, we need to compute its eigenvalues in order to evaluate its Rényi entropy. Considering that the dimension of \mathcal{H}_X is 2^L the computational time grows, in principle, exponentially with the size of the subsystem.

As we will see in the next section, there is an algorithm due to Peschel [13], that allows to reduce the exponential growth to a potential one.

III. WICK DECOMPOSITION

Wick theorem is a key ingredient in the perturbative expansion of quantum field theory. It implies that the correlation function of $2J$ points can be decomposed into the correlation

functions of the different possible pairings of the points.

We say that a state with density matrix ρ satisfies the Wick decomposition property if the correlation of an odd number of points is zero and for every J we have

$$\text{Tr}(\rho d_1 \dots d_{2J}) = \frac{1}{J!} \sum_{\sigma \in S'_{2J}} \prod_{j=1}^J (-1)^{|\sigma|} \text{Tr}(\rho d_{\sigma(2j-1)} d_{\sigma(2j)}),$$

where

$$d_j = \sum_{n=1}^N \alpha_j(n) a_n + \beta_j(n) a_n^\dagger$$

is any linear combination of creation and annihilation operators,

$$S'_{2J} = \{\sigma \in S_{2J} \mid \sigma(2j-1) < \sigma(2j), j = 1, \dots, J\}$$

is the set of permutations that preserve the order in every pair and $|\sigma|$ is the signature of σ . It is interesting to notice that if the original density matrix of our system ρ satisfies such a property, then the reduced density matrix ρ_X also admits the Wick decomposition, as one can trivially check.

In the following we will further assume that ρ preserves the total fermionic number and therefore $\text{Tr}(\rho a_n a_m) = \text{Tr}(\rho a_n^\dagger a_m^\dagger) = 0$. This property is also inherited by the reduced density matrix.

In order to proceed we must solve the inverse problem. That is, given the correlation matrix

$$C_{nm} = \text{Tr}(\rho a_n^\dagger a_m)$$

and assuming that the state satisfies the Wick decomposition property, determine the density matrix.

To achieve this goal we diagonalise the correlation matrix that has real eigenvalues in the interval $[0, 1]$. Denote by $\{\phi_1, \dots, \phi_N\}$ the orthonormal basis of eigenvectors with respective eigenvalues μ_l , $l = 1, \dots, N$, and by

$$c_l = \sum_{n=1}^N \phi_l(n) a_n$$

the basis of annihilation operators for which the correlation matrix is diagonal. They satisfy, of course, the canonical anticommutation relations. We shall consider three disjoint sets in $\{1, \dots, N\}$: E_1 which contains the indices l for which $\mu_l = 0$, E_2 that contains the

indices such that $\mu_l = 1$ and finally E_3 that contains the rest of indices, i.e. those with $0 < \mu_l < 1$.

Consider first the set E_1 . It is clear that if $\text{Tr}(\rho c_p^\dagger c_p) = 0$, i.e. $p \in E_1$ and we denote by P_p the orthogonal projector into the image of c_p , then we can write $\rho = Q P_p$. By the same token if $\mu_q = 1$ then $\rho = Q'(1 - P_q)$. Following these remarks, we introduce the ansatz for the density matrix

$$\rho = K e^{-h} \prod_{p \in E_1} P_p \prod_{q \in E_2} (1 - P_q),$$

with $h = \sum_{l \in E_3} \epsilon_l c_l^\dagger c_l$ and K the normalisation constant. It is easy to see that ρ satisfies the Wick decomposition property, the eigenspaces with eigenvalues 0 and 1 in the correlation matrix match and, as we will show below, with the adequate choice of h we can also account for the other eigenvalues.

If ρ describes completely the state of the system $\text{Tr}(\rho) = 1$. Using this fact, we can determine the normalisation constant

$$K = \frac{1}{\prod_{l \in E_3} (1 + e^{-\epsilon_l})}$$

Therefore, the normalised ρ is

$$\rho = \prod_{p \in E_1} P_p \prod_{q \in E_2} (1 - P_q) \prod_{l \in E_3} \frac{e^{-\epsilon_l c_l^\dagger c_l}}{1 + e^{-\epsilon_l}}. \quad (6)$$

In order to determine the coefficients ϵ_l we compute

$$\text{Tr}(\rho c_l^\dagger c_l) = \frac{1}{1 + e^{\epsilon_l}},$$

and, then, we can relate the eigenvalues of the correlation matrix to those of h ,

$$\epsilon_l = \log \frac{1 - \mu_l}{\mu_l}, \quad \text{for } 0 < \mu_l < 1. \quad (7)$$

If, for a moment, we assume that E_1 and E_2 are empty, i. e. $0 < \mu_l < 1$ for any l , then there is a simple relation between h and the correlation matrix in terms of the original creation and annihilation operator basis. In fact, writing

$$h = \sum_{n,m=1}^N M_{nm} a_n^\dagger a_m$$

and denoting by $C = (C_{nm})$ and $M = (M_{nm})$ the corresponding matrices one has

$$M = \log(C^{-1} - I) \Leftrightarrow C = (e^M + I)^{-1}$$

Note that the magic of this procedure is that we have determined the density matrix, of dimension 2^N , through a function of the correlation matrix of dimension N . This fact allows us to go to larger values of N without exhausting the computational capabilities. Note, however, that this dramatic simplification of the problem relies in the fact that the density matrix is supposed to satisfy the Wick decomposition property, a fact that must be checked in every case. One example that satisfies the Wick decomposition theorem is the density matrix associated to the Slater determinant $|\Psi_{\mathcal{K}}\rangle$ in (4). This case corresponds to $E_3 = \emptyset$, $E_2 = \mathcal{K}$ and E_1 its complementary \mathcal{K}^c . Therefore, if our state of interest ρ satisfies the Wick decomposition property, according to the previous discussion, also the reduced density matrix ρ_X has such a property and hence the previous considerations will be relevant for us.

Once we have determined the density matrix we can compute its Rényi entropy and express it in terms of the eigenvalues of the correlation matrix. In fact, using (6) and (7) we have

$$\text{Tr}(\rho^\alpha) = \prod_{l \in E_3} \frac{1 + e^{-\alpha \epsilon_l}}{(1 + e^{-\epsilon_l})^\alpha} = \prod_{l=1}^N [(1 - \mu_l)^\alpha + \mu_l^\alpha],$$

where in the last equality the product to *all* the eigenvalues of C (also those that are 0 or 1) can be included without any change in the result. Therefore

$$S_\alpha = \frac{1}{1 - \alpha} \sum_{l=1}^N \log[(1 - \mu_l)^\alpha + \mu_l^\alpha], \quad (8)$$

expresses the Rényi entropy of the density matrix ρ in terms of its correlation. In matrix form we have

$$S_\alpha = \frac{1}{1 - \alpha} \text{Tr} \log[(I - C)^\alpha + C^\alpha].$$

When $\alpha \rightarrow 1$, that is the von Neumann entropy, the previous formulae lead to

$$S_1 = - \sum_{l=1}^N [(1 - \mu_l) \log(1 - \mu_l) + \mu_l \log \mu_l],$$

or

$$S_1 = - \text{Tr} [(I - C) \log(I - C) + C \log C].$$

The discussion has been restricted to our case of interest in which ρ preserves the total fermionic number and, therefore, $\text{Tr}(\rho a_n^\dagger a_m^\dagger) = 0$. However a similar result is obtained in the general case, with the particularity that the transformation to the new creation and annihilation operators c_l^\dagger, c_l that diagonalises the correlation matrix is of Bogoliubov type, and the previous expressions that involve the correlation matrix should be adequately modified [13].

IV. CORRELATION MATRIX OF THE TOEPLITZ TYPE

In order to be able to analytically compute the entropy of the reduced system (in the large N limit) it will be crucial that the correlation matrix is of the Toeplitz type, i.e.

$$C_{nm} = \xi_{n-m}.$$

Evidently, this property is a consequence of the translational invariance of the system. We will see now under which conditions it holds.

Let us consider a state like in (4)

$$|\Psi_{\mathcal{K}}\rangle = \prod_{k \in \mathcal{K}} b_k^\dagger |0\rangle,$$

where we assume that b -operators

$$b_k = \sum_{n=1}^N \varphi_k(n) a_n, \quad k = 1 - N/2, \dots, N/2$$

satisfy the canonical anticommutation relations. This fact implies that the matrix built with these coefficients, $\varphi_k(n)$, is unitary (i.e. they form an orthonormal basis). Then the inverse transformation is

$$a_n = \sum_{k=1-N/2}^{N/2} \varphi_k^*(n) b_k.$$

In the previous section we have shown that the Rényi entropy of a subsystem of the chain can be obtained from the correlation matrix,

$$C_{nm} = \langle \psi | a_n^\dagger a_m | \psi \rangle.$$

In particular, for the state $|\Psi_{\mathcal{K}}\rangle$, we find that the elements of the correlation matrix are

$$C_{nm} = \sum_{k \in \mathcal{K}} \varphi_k(n) \varphi_k^*(m). \quad (9)$$

But, if we demand that C_{nm} is a Toeplitz matrix the $\varphi_k(n)$ must satisfy

$$\varphi_k(n)\varphi_k^*(m) = \xi_k(n-m). \quad (10)$$

That is, the product $\varphi_k(n)\varphi_k^*(m)$ must be invariant under translations in n . The only functions which constitute an orthonormal basis and satisfy (10) are

$$\varphi_k(n) = \frac{1}{\sqrt{N}} e^{2\pi i k n / N},$$

i.e. the coefficients of the discrete Fourier transform. In this case the correlation matrix reads

$$C_{nm} = \frac{1}{N} \sum_{k \in \mathcal{K}} e^{2\pi i k (n-m) / N}. \quad (11)$$

In the following section it will be convenient to use $V = 2C - I$ instead of the correlation matrix. In our case it has the following expression

$$V_{nm} = \frac{1}{N} \left(\sum_{k \in \mathcal{K}} e^{2\pi i k (n-m) / N} - \sum_{k \notin \mathcal{K}} e^{2\pi i k (n-m) / N} \right). \quad (12)$$

Coming back to the correlation matrix we would like to study some of its transformation properties that result in the invariance of the entropy.

1. Translational invariance of the entropy in the coordinate space (a -particles), which comes from the fact that C is a Toeplitz matrix.
2. Translational invariance in the momentum space (b -modes) of the state. Let \mathcal{K} be a particular configuration of occupied modes and let $\mathcal{K}' = \mathcal{K} + \Delta = \{k + \Delta | k \in \mathcal{K}\}$. The correlation matrix for \mathcal{K}' is

$$C'_{nm} = \frac{1}{N} \sum_{k' \in \mathcal{K}'} e^{2\pi i k' (n-m) / N}$$

Changing the variable of the sum, $k = k' - \Delta$

$$C'_{nm} = \frac{1}{N} \sum_{k \in \mathcal{K}' - \Delta} e^{2\pi i (k+\Delta)(n-m) / N} = e^{2\pi i n \Delta / N} C_{nm} e^{-2\pi i m \Delta / N} \quad (13)$$

Defining now the unitary matrix U

$$U_{nm} = e^{-2\pi i n \Delta / N} \delta_{nm}$$

we can rewrite the expression (13)

$$C'_{nm} = (U^\dagger C U)_{nm}$$

Therefore C' results from applying a unitary transformation to C , so that their eigenvalues are the same and the associated entropy is equal.

3. Invariance under complementarity in b -space. Consider a particular configuration \mathcal{K} and call \mathcal{K}^c its complementary set. The correlation matrix for \mathcal{K}^c is

$$C_{nm}^c = \sum_{k \in \mathcal{K}^c} \varphi_k(n) \varphi_k^*(m) = \frac{1}{N} \sum_{k \in \mathcal{K}^c} e^{2\pi i k(n-m)/N}$$

Using the fact $\{\varphi_k(n)\}$ is an orthonormal basis

$$\sum_{k=1}^N \varphi_k(n) \varphi_k^*(m) = \delta_{nm}$$

we can decompose the last sum into two pieces

$$\delta_{nm} = \sum_{k \in \mathcal{K}} \varphi_k(n) \varphi_k^*(m) + \sum_{k \in \mathcal{K}^c} \varphi_k(n) \varphi_k^*(m) = C_{nm} + C_{nm}^c.$$

Therefore, the eigenvalues of C_{nm}^c are $\mu_l^c = 1 - \mu_l$. Inserting them into (8) we find that the entropies of the states determined by \mathcal{K}^c and \mathcal{K} are the same.

It is interesting to remark that these properties reflect the duality between the representation in coordinate space a_n and in momentum space b_k . In fact in both scenarios we have translational invariance of the entropy and also invariance under complementarity.

V. ENTANGLEMENT ENTROPY FOR A SINGLE BLOCK

Suppose that the total correlation matrix of the chain is Toeplitz and a subsystem X which is a single block of L contiguous sites in the coordinate space. In this case, the correlation matrix of the subsystem, which we denote by $C(X)$, is a Toeplitz matrix as well. Using the properties of the Toeplitz matrices, the existence of a generating function and the Fisher-Hartwig conjecture, we can find how the entropy scales with the size of X in the thermodynamic limit.

If we denote by $v_l = 2\mu_l - 1$ the eigenvalues of the matrix $V(X) = 2C(X) - I_L$ (which is a Toeplitz matrix too), the Rényi entropy (8) can be written

$$S_\alpha(X) = \frac{1}{1-\alpha} \sum_{l=1}^L \log \left[\left(\frac{1+v_l}{2} \right)^\alpha + \left(\frac{1-v_l}{2} \right)^\alpha \right]. \quad (14)$$

It will be convenient to transform the sum in the previous expression into a complex integral on a contour that encloses the eigenvalues of $V(X)$. To that end we introduce the function

$$f_\alpha(x, y) = \frac{1}{1-\alpha} \log \left[\left(\frac{x+y}{2} \right)^\alpha + \left(\frac{x-y}{2} \right)^\alpha \right],$$

and applying the Cauchy's residue theorem we can rewrite the Rényi entropy (14) in terms of a complex integral:

$$S_\alpha(X) = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{2\pi i} \oint_{\mathcal{C}} f_\alpha(1+\varepsilon, \lambda) \frac{d \log D_L(\lambda)}{d\lambda} d\lambda, \quad (15)$$

where $D_L(\lambda)$ is the determinant of $\lambda I_L - V(X)$,

$$D_L(\lambda) = \prod_{l=1}^L (\lambda - v_l),$$

and the contour \mathcal{C} surrounds all the eigenvalues of V which are the poles of the integrand. The contour of integration, the poles and the cuts are depicted in the figure.

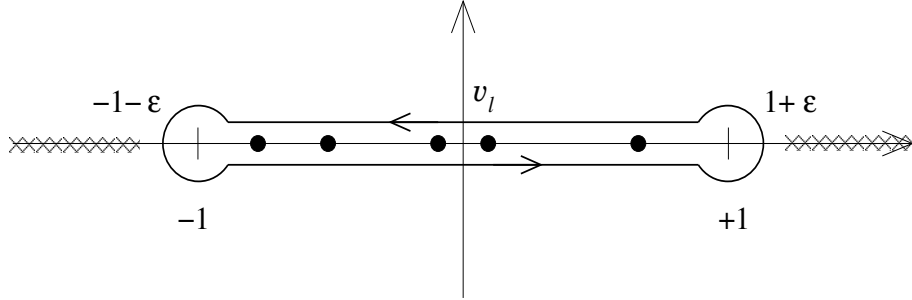


FIG. 1: Contour of integration, cuts and poles for the computation of $S_\alpha(X)$. The cuts for the function f_α extend to $\pm\infty$.

A state $|\Psi_{\mathcal{K}}\rangle$ is characterised by the set of occupied modes \mathcal{K} . In the thermodynamic limit this can be approximated by an occupation density, so we describe the state through a periodic function $g(\theta)$ that takes values in the interval $[-1, 1]$ and is defined by

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} F(\theta) g(\theta) d\theta = \lim_{N \rightarrow \infty} \frac{1}{N} \left[\sum_{k \in \mathcal{K}} F\left(\frac{2\pi k}{N}\right) - \sum_{k \notin \mathcal{K}} F\left(\frac{2\pi k}{N}\right) \right],$$

where the equality should hold for any continuous function F . Notice that $g(\theta) = 1$ if the modes with momenta around $k_\theta = N\theta/(2\pi)$ are all occupied and $g(\theta)$ is -1 if they are empty. Intermediate values represent the occupation of only a fraction of the b -modes with momenta near k_θ .

Now, we can replace in (12) the sum with an integral

$$V_{nm} = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(\theta) e^{i(n-m)\theta} d\theta.$$

The kind of occupation densities we will be interested in are piecewise constant functions. If we denote by $\theta_1, \dots, \theta_R$ the discontinuity points,

$$g(\theta) = t_r, \quad \theta_{r-1} \leq \theta < \theta_r. \quad (16)$$

Note that the ground state of a quadratic, translational invariant Hamiltonian with short range interactions, corresponds to t_r taking the values $+1$ or -1 . Later we will discuss the physical interpretation of more general occupation densities.

Following Jin and Korepin [15], we use the Fisher-Hartwig conjecture to compute the determinant D_L [19, 20]. We express $\tilde{g}(\theta) = \lambda - g(\theta)$ in the form

$$\tilde{g}(\theta) = \psi(\theta) \prod_{r=1}^R \tau_r(\theta - \theta_r),$$

where

$$\psi(\theta) = \prod_{r=1}^R (\lambda - t_{r-1})^{\frac{\theta_r - \theta_{r-1}}{2\pi}}$$

and the discontinuities are taken into account by the functions

$$\tau_r(\theta) = e^{-i\beta_r(\pi - \theta)}, \quad \theta \in [0, 2\pi),$$

that have a jump at $\theta = 0$, while

$$\beta_r = -\frac{1}{2\pi i} \log \left(\frac{\lambda - t_{r-1}}{\lambda - t_r} \right).$$

The Fisher-Hartwig conjecture (which has been proven for our case [14]) states that up to a factor that goes to 1 when $L \rightarrow \infty$, the determinant of our Toeplitz matrix, D_L , can be approximated by

$$D_L \approx (F[\psi])^L \left(\prod_{r=1}^R L^{-\beta_r^2} \right) E[\{\beta_r\}, \{\theta_r\}],$$

where $F[\psi] = e^{\frac{1}{2\pi} \int_0^{2\pi} \log(\psi(\theta)) d\theta}$ and

$$E[\{\beta_r\}, \{\theta_r\}] = \prod_{r=1}^R G(1 + \beta_r) G(1 - \beta_r) \prod_{1 \leq r \neq r' \leq R} (1 - e^{i(\theta_r - \theta_{r'})})^{\beta_r \beta_{r'}} \quad (17)$$

with $G(z)$ the Barnes G-function. The logarithmic derivative of D_L is

$$\frac{d \log D_L(\lambda)}{d\lambda} = \frac{d \log F[\psi]}{d\lambda} L - \sum_{r=1}^R \frac{d\beta_r^2}{d\lambda} \log L + \frac{\log E}{d\lambda} + \dots,$$

where the dots stand for terms that vanish in the large L limit. Inserting this expression into (15) we can compute the entropy for large L . Namely

$$S_\alpha(X) = A_\alpha L + B_\alpha \log L + C_\alpha + \dots \quad (18)$$

and our next task is to compute the coefficients in the expansion.

With respect to the linear term A_α , if we consider that ψ does not depend on θ , we have $F[\psi] = \psi$. Taking its logarithmic derivative, introducing it in (15) and applying the Cauchy's residue theorem we obtain

$$A_\alpha = \frac{1}{2\pi} \int_{-\pi}^{\pi} f_\alpha(1, g(\theta)) d\theta. \quad (19)$$

As for the coefficient of the logarithmic term B_α , we have

$$B_\alpha = -\frac{1}{2\pi i} \sum_{r=1}^R \lim_{\varepsilon \rightarrow 0^+} \oint_{\mathcal{C}} f_\alpha(1 + \varepsilon, \lambda) \frac{d\beta_r^2}{d\lambda} d\lambda,$$

where the poles and cuts of the r -th term in the sum are represented in the figure.

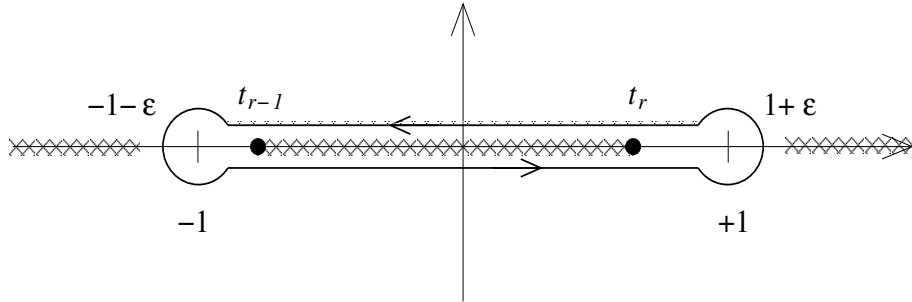


FIG. 2: Contour of integration, cuts and poles for the computation of B_α .

This integral has been considered before in the literature. The usual strategy to compute it goes through the decomposition of the contour into different pieces with divergent

integrals. After an annoying computation it is shown that the divergences cancel to render a finite result. See [15] for the original work and [17] for a recent application. We propose a new strategy that leads directly to the finite result in a simpler way. It consists in performing an integration by parts, so that

$$B_\alpha = \frac{1}{2\pi i} \sum_{r=1}^R \lim_{\varepsilon \rightarrow 0^+} \oint_{\mathcal{C}} \frac{df_\alpha(1+\varepsilon, \lambda)}{d\lambda} \beta_r^2 d\lambda.$$

Now a straightforward computation of the integral along \mathcal{C} gives

$$B_\alpha = \frac{1}{2\pi i} \sum_{r=1}^R \frac{1}{4\pi^2} \int_{t_{r-1}}^{t_r} \frac{df_\alpha(1, \lambda)}{d\lambda} \left[\left(\log \left| \frac{\lambda - t_r}{\lambda - t_{r-1}} \right| + i\pi \right)^2 - \left(\log \left| \frac{\lambda - t_r}{\lambda - t_{r-1}} \right| - i\pi \right)^2 \right] d\lambda,$$

and at last

$$B_\alpha = \frac{1}{2\pi^2} \sum_{r=1}^R \int_{t_{r-1}}^{t_r} \frac{df_\alpha(1, \lambda)}{d\lambda} \log \left| \frac{\lambda - t_r}{\lambda - t_{r-1}} \right| d\lambda. \quad (20)$$

So, we write the logarithmic coefficient as an integral that, in general, should be determined numerically. In the next section we will give some examples in which B_α is analytically computed.

Finally, we must obtain the finite contribution C_α . Proceeding as before we have

$$C_\alpha = \frac{1}{2\pi i} \lim_{\varepsilon \rightarrow 0^+} \oint_{\mathcal{C}} f_\alpha(1+\varepsilon, \lambda) \left[\sum_{r=1}^R \frac{d}{d\lambda} \log[G(1+\beta_r)G(1-\beta_r)] + \sum_{1 \leq r \neq r' \leq R} \log(1 - e^{i(\theta_r - \theta_{r'})}) \frac{d}{d\lambda} (\beta_r \beta_{r'}) \right] d\lambda$$

We have to deal with two different integrals. The first one reads

$$\begin{aligned} I_\alpha(r) &= \frac{1}{2\pi i} \lim_{\varepsilon \rightarrow 0^+} \oint_{\mathcal{C}} f_\alpha(1+\varepsilon, \lambda) \frac{d}{d\lambda} \log[G(1+\beta_r)G(1-\beta_r)] d\lambda \\ &= \frac{-1}{2\pi i} \lim_{\varepsilon \rightarrow 0^+} \oint_{\mathcal{C}} \frac{df_\alpha(1+\varepsilon, \lambda)}{d\lambda} \log[G(1+\beta_r)G(1-\beta_r)] d\lambda \end{aligned} \quad (21)$$

where we have performed an integration by parts. The cuts in the complex plane for the above integral are again those of fig. 2. Therefore, after integrating along the contour we get

$$I_\alpha(r) = \frac{1}{2\pi i} \int_{t_{r-1}}^{t_r} \frac{df_\alpha(1, \lambda)}{d\lambda} \log \left[\frac{G(1+\beta_r^-)G(1-\beta_r^-)}{G(1+\beta_r^+)G(1-\beta_r^+)} \right] d\lambda$$

where

$$\beta_r^\pm = i\omega_r(\lambda) \pm \frac{1}{2}, \quad \text{with} \quad \omega_r(\lambda) = \frac{1}{2\pi} \log \left| \frac{\lambda - t_r}{\lambda - t_{r-1}} \right|.$$

Note that $\beta_r^+ = \beta_r^- + 1$, so applying the property of the Barnes G-function $G(z+1) = \Gamma(z)G(z)$, where Γ is the Euler gamma function, we finally obtain

$$I_\alpha(r) = \frac{1}{2\pi i} \int_{t_{r-1}}^{t_r} \frac{df_\alpha(1, \lambda)}{d\lambda} \log \left[\frac{\Gamma(1/2 - i\omega_r(\lambda))}{\Gamma(1/2 + i\omega_r(\lambda))} \right] d\lambda. \quad (22)$$

The computation of the second integral goes along similar lines. Define

$$\begin{aligned} J_\alpha(r, r') &= -\frac{1}{2\pi i} \lim_{\varepsilon \rightarrow 0^+} \oint_{\mathcal{C}} f_\alpha(1 + \varepsilon, \lambda) \frac{d(\beta_r \beta_{r'})}{d\lambda} d\lambda \\ &= \frac{1}{2\pi i} \lim_{\varepsilon \rightarrow 0^+} \oint_{\mathcal{C}} \frac{df_\alpha(1 + \varepsilon, \lambda)}{d\lambda} \beta_r \beta_{r'} d\lambda, \end{aligned}$$

where, again, we find useful to perform an integration by parts to achieve the cancellation of divergences. There are two cuts in the region inside the integral contour going from t_{r-1} to t_r and from $t_{r'-1}$ to $t_{r'}$ respectively. The integral should be decomposed into different regions corresponding to the different cuts and computed carefully. But, considering that we only meet harmless logarithmic singularities, we can appropriately group the different terms to obtain

$$J_\alpha(r, r') = K_\alpha(r, r') + K_\alpha(r', r)$$

where

$$K_\alpha(r, r') = \frac{1}{4\pi^2} \int_{t_{r-1}}^{t_r} \frac{df_\alpha(1, \lambda)}{d\lambda} \log \left| \frac{\lambda - t_{r'}}{\lambda - t_{r'-1}} \right| d\lambda$$

Therefore, putting all together we have

$$C_\alpha = \sum_{r=1}^R I_\alpha(r) - \sum_{1 \leq r \neq r' \leq R} \log[2 - 2\cos(\theta_r - \theta_{r'})] K_\alpha(r, r') \quad (23)$$

To our knowledge, this is the first time that such an explicit expression of the constant term, for general values of t_r , appears in the literature.

Note that if our state has $g(\theta) = \pm 1$, with a finite number of discontinuities, the entropy of X scales with $\log L$ because in this case the coefficient of the linear term vanishes. It has been shown in [7] that these configurations correspond to the ground state of a Hamiltonian with local interactions. On the other hand, if there are intervals with $g(\theta) \neq \pm 1$ the entropy exhibits both linear and logarithmic contributions. It has been proposed that these configurations correspond, in general, to the ground state of a non-local Hamiltonian [7]. In section VII we will carry out a thorough discussion on the connection of our kind of states, its entanglement entropy and quadratic Hamiltonians for chains and ladders.

VI. NUMERICAL RESULTS

In this section we present the results for the Rényi entanglement entropy of a single interval of length L , when $\alpha \rightarrow 1$ (von Neumann entropy) and $\alpha = 2$. We perform the computation using the analytic expressions obtained in the previous section for the expansion in L and compare with the numerical results. As we discussed before, thanks to the Wick decomposition property [13], we can easily cover values of $L = 10^3$, in the numeric computation (note that ρ_X acts on Hilbert space of dimension 2^{1000} which is impossible to deal with in any computer).

We consider three different pure states, each one characterised by a set \mathcal{K} of occupied b -modes. In the thermodynamic limit they are described by its occupation density. With these three states we can check different aspects of the analytic expressions obtained before.

State 1: half of the b -modes, corresponding to the lowest absolute value of the momenta, are occupied, while the others are empty. The state can be represented by $(0 \dots 01 \dots 11 \dots 10 \dots 0)$ where every digit represents the occupation -1- or not -0- of the mode of the corresponding momentum k . The occupation density is

$$g(\theta) = \begin{cases} -1, & \theta \in [-\pi, -\pi/2) \cup [\pi/2, \pi], \\ 1, & \theta \in [-\pi/2, \pi/2). \end{cases}$$

Note that this is precisely the ground state of the Tight Binding Model with the local periodic Hamiltonian

$$H = -T \sum_{n=1}^N a_n^\dagger (a_{n-1} + a_{n+1}), \quad (24)$$

and $T > 0$. Since it is invariant under translations it is diagonalised by the Fourier transformation so that its eigenstates are $|\Psi_{\mathcal{K}}\rangle = \prod_{k \in \mathcal{K}} b_k^\dagger |0\rangle$

$$H |\Psi_{\mathcal{K}}\rangle = \sum_{k \in \mathcal{K}} \Lambda_k |\Psi_{\mathcal{K}}\rangle; \quad \Lambda_k = -2T \cos\left(\frac{2\pi k}{N}\right)$$

State 2: b -modes with momenta $|k| > N/4$ are empty while those with $|k| < N/4$ are occupied alternatively. This can be represented by $(0 \dots 0 10 \dots 10 0 \dots 0)$. Then

the occupation density is

$$g(\theta) = \begin{cases} -1, & \theta \in [-\pi, -\pi/2) \cup [\pi/2, \pi], \\ 0, & \theta \in [-\pi/2, \pi/2]. \end{cases}$$

State 3: for $|k| > N/4$ all b -modes are empty, while for the other half there are three out of four occupied, i. e. $(0 \dots 0 \ 1110 \dots 1110 \ 0 \dots 0)$. Therefore, the occupation density is

$$g(\theta) = \begin{cases} -1, & \theta \in [-\pi, -\pi/2) \cup [\pi/2, \pi], \\ 1/2, & \theta \in [-\pi/2, \pi/2]. \end{cases}$$

In our numerical calculations we take the thermodynamic limit and compute the entropies of a single block with a length varying from $L = 10$ to $L = 1000$ sites. Dots in figures 3, 4 and 5 represent the numerical results, while the continuous line stands for the analytic results for the large L expansion.

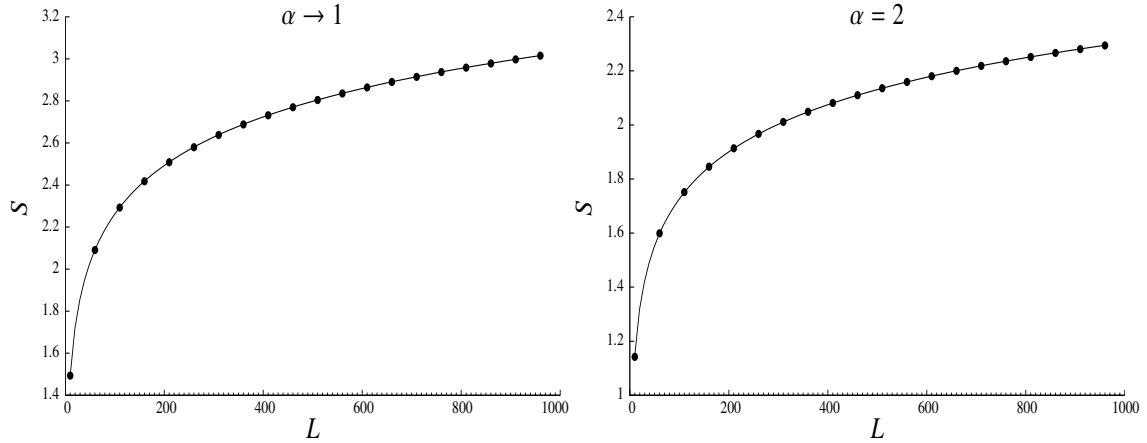


FIG. 3: Entropy when $\alpha \rightarrow 1$ (left panel) and $\alpha = 2$ (right panel) as a function of the length L of the block when the chain is in the **state 1**. The dots are the numerical values while the continuous line represents the asymptotic expansion (18) with $A_\alpha = 0$, $B_1 = 1/3$, $C_1 = 0.726067$ and $B_2 = 1/4$, $C_2 = 0.577336$ respectively.

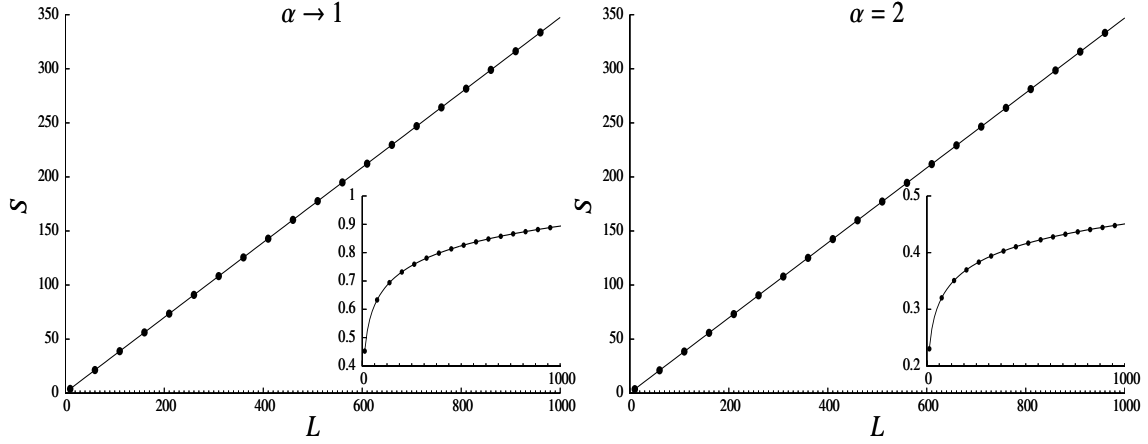


FIG. 4: Entropy when $\alpha \rightarrow 1$ (left panel) and $\alpha = 2$ (right panel) for the **state 2**. The dots are the numerical values and the continuous line represents the Fisher-Hartwig expansion (18) with the coefficients of table 1. In the insets we plot the entropy subtracting the linear contribution to reveal the logarithmic term.

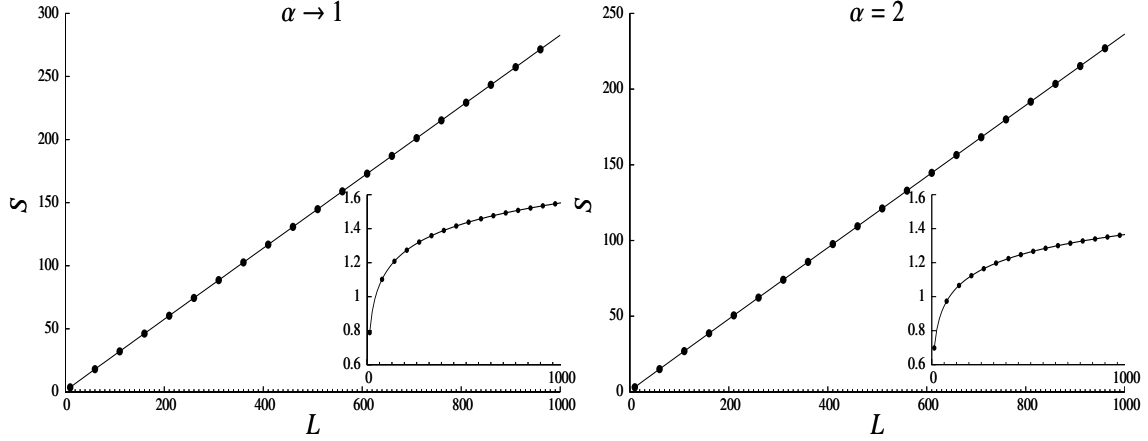


FIG. 5: Entropy when $\alpha \rightarrow 1$ (left panel) and $\alpha = 2$ (right panel) in the **state 3**. The dots are the numerical values while the continuous line represents the Fisher-Hartwig expansion (18) with the coefficients of table 1. In the insets we plot the entropy subtracting the linear contribution.

The table I summarises the numerical values of A_α , B_α and C_α that we get using the expressions found in the previous section for these particular states. We compare them to those obtained by fitting the numerical entropies, computed from the correlation matrix of the subsystem.

$\alpha \rightarrow 1$	A_1		B_1		C_1	
State	F-H	num.	F-H	num.	F-H	num.
1	0	0	1/3	0.333343	0.726067	0.726600
2	0.3465735	0.346574	0.100660	0.100669	0.220813	0.220768
3	0.2811676	0.281168	0.175015	0.175019	0.385367	0.385460

$\alpha = 2$	A_2		B_2		C_2	
State	F-H	num.	F-H	num.	F-H	num.
1	0	0	1/4	0.251098	0.577336	0.570234
2	0.3465735	0.346574	0.050330	0.050314	0.114183	0.114270
3	0.2350018	0.235001	0.152477	0.152875	0.349182	0.347217

TABLE I: The “F-H” columns collect the predicted values of A_α , B_α and C_α using the Fisher-Hartwig conjecture when $\alpha \rightarrow 1$ (upper table) and $\alpha = 2$ (lower table). The corresponding “num.” columns contain the value of these coefficients when we fit the numerical entropies with the expansion (18).

The agreement between the outcomes is excellent. Note that when the linear term is nonzero, it provides the best fit to the numerical entropies because it dominates. On the contrary, the adjustment of the finite term is the poorest. From these results we can conclude that the large L expansion (18) works rather well from lengths of $L = 10$ sites. On the other hand, one may ask how our results are affected by finite-size effects. In this sense we have performed numerical simulations for finite N and we can conclude that the expansion works reasonably well (when $L \in [10, 1000]$) from around $N = 10^4$.

State 1 is specially interesting, as it corresponds to the ground state of (24) that is a critical (gapless) theory. The entropy grows logarithmically as it is predicted from conformal field theory (3) with central charge $c = 1$. The comparison with the expression for the coefficient of the logarithmic term (20) and (3) leads to the following integral identity,

$$\frac{1}{1-\alpha} \int_{-1}^1 \log \left[\left(\frac{1+x}{2} \right)^\alpha + \left(\frac{1-x}{2} \right)^\alpha \right] \frac{dx}{1-x^2} = \frac{\pi^2}{12} \frac{1+\alpha}{\alpha} \quad (25)$$

which can be analytically derived with the change of variables $x = (t-1)/(t+1)$ that also reveals the relationship with the dilogarithm function.

Concerning the state 2, first note that its linear coefficient does not depend on α . Actually it is easy to compute to give

$$A_\alpha = \frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} f_\alpha(1, 0) d\theta = \log(2)/2,$$

that agrees with the numerical results. In addition, for this configuration the logarithmic coefficient for integer α can be analytically obtained. It has the expression

$$B_\alpha = \frac{\alpha + 1}{24\alpha} - \frac{1}{2\pi^2(\alpha - 1)} \sum_{n=1}^{\alpha} \left(\log \sin \frac{(2n - 1)\pi}{2\alpha} \right)^2,$$

for $\alpha \geq 2$, while for $\alpha = 1$ is

$$B_1 = \frac{1}{8} - \frac{1}{2} \left(\frac{\log 2}{\pi} \right)^2,$$

values that agree with the numerical ones that appear in the table.

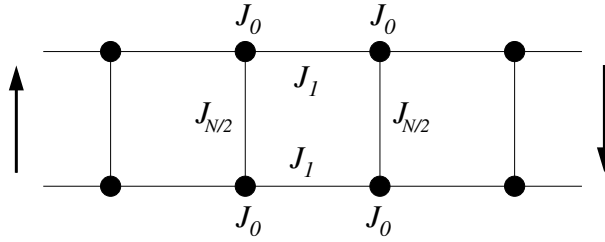


FIG. 6: Representation of the fermionic ladder with the couplings of the Hamiltonian of (26). The upper row contains the sites from 1 to $N/2$ of the chain and the lower one those from $N/2 + 1$ to N , both from left to right. The ends of the ladder are joined with an inversion as it is indicated by the arrows, forming, therefore, a Moebius strip.

As it is discussed in [7], states whose entropy grows linearly with the size of the interval may correspond to the vacuum of a non-local Hamiltonian. This can be shown to hold in our case. In fact, consider the simple Hamiltonian

$$H = \sum_n (J_0 a_n^\dagger a_n + J_1 a_n^\dagger a_{n+1} + J_{N/2} a_n^\dagger a_{n+N/2}) + h.c., \quad (26)$$

that corresponds to a fermionic ladder as it is depicted in the figure 6 (note that one must perform an inversion when joining the two ends forming a Moebius strip rather than a periodic ladder). If we take the coupling constants

$$J_{N/2} = J_0 > 0, \quad J_1 = -2J_0,$$

the ground state is precisely the state 2.

A similar result is obtained for state 3. If we consider the Hamiltonian

$$H = \sum_n (J_0 a_n^\dagger a_n + J_1 a_n^\dagger a_{n+1} + J_{N/4} a_n^\dagger a_{n+N/4} + J_{N/2} a_n^\dagger a_{n+N/2}) + h.c.,$$

with

$$J_{N/2} = J_0 > 0, \quad J_{N/4} = 2J_0 \quad \text{and} \quad J_1 = -4J_0,$$

its vacuum is state 3.

Note that our results follow the *rule of thumb* according to which the ground state entanglement entropy grows like the number of bonds that are broken when isolating the subsystem. As it is evident from the figure 6, the number of bonds that we break when isolating a connected subchain depends linearly on the size of the interval, which explains the presence of a linear term in the expansion of the entanglement entropy. The same is true for state 3, while state 1, that is the ground state of a local Hamiltonian, does not have this property.

VII. FERMIONIC CHAINS AND LADDERS

In this section we will try to gain physical insights from the previous results and extend them to more general states. In order to do that, and as a continuation of the discussion in the former section (see also [7]), it will be useful to consider $|\Psi_{\mathcal{K}}\rangle$ as the ground state of a free, homogeneous Hamiltonian of the following form

$$H = \sum_{n=1}^N \sum_{j=1}^{N/2} J_j a_n^\dagger a_{n+j} + h.c.,$$

where $a_{n+N} = a_n$ and the coupling constants J_j may take complex values. Of course, due to the translational invariance of the Hamiltonian the eigenstates are of the general form introduced in (4)

$$|\Psi_{\mathcal{K}}\rangle = \prod_{k \in \mathcal{K}} b_k^\dagger |0\rangle$$

with eigenvalue

$$E_{\mathcal{K}} = \sum_{k \in \mathcal{K}} \Lambda_k$$

where the dispersion relation is given by

$$\Lambda_k = \sum_{j=1}^{N/2} J_j e^{2\pi i k j / N} + c.c.$$

The ground state of this Hamiltonian is therefore

$$|GS\rangle = \prod_{\Lambda(k) < 0} b_k^\dagger |0\rangle$$

We consider two types of Hamiltonians according to the behaviour of the couplings with j . We shall say that the Hamiltonian is local in the chain if the couplings are rapidly decaying in j , i.e.

$$\lim_{j \rightarrow \infty} J_j j^\gamma = 0, \text{ for any real } \gamma.$$

In this case [7] the thermodynamic limit of the dispersion relation

$$\Lambda(\theta) = \sum_{j=1}^{\infty} J_j e^{i\theta j} + c.c.,$$

is a smooth function that generically has a finite (even) number of zeros where Λ changes its sign, call this number ν . A typical example with $\nu = 4$ is represented in the upper half of Fig. 7 A.

The occupation density for the ground state will be given by

$$g(\theta) = \begin{cases} 1, & \text{if } \Lambda(\theta) < 0 \\ -1, & \text{if } \Lambda(\theta) > 0, \end{cases} \quad (27)$$

which is a piecewise constant function with values ± 1 . Therefore, the linear term of the entanglement entropy is absent and we get

$$S_\alpha(X) = \frac{1+\alpha}{\alpha} \frac{\nu}{12} \log L + C_\alpha,$$

where the constant C_α depends on the precise location of the discontinuities. We represent in Fig. 7 A (lower half) the occupation density for the particular dispersion relation plotted on top it.

We would like to highlight some features of this result, as they will be useful for our later discussion.

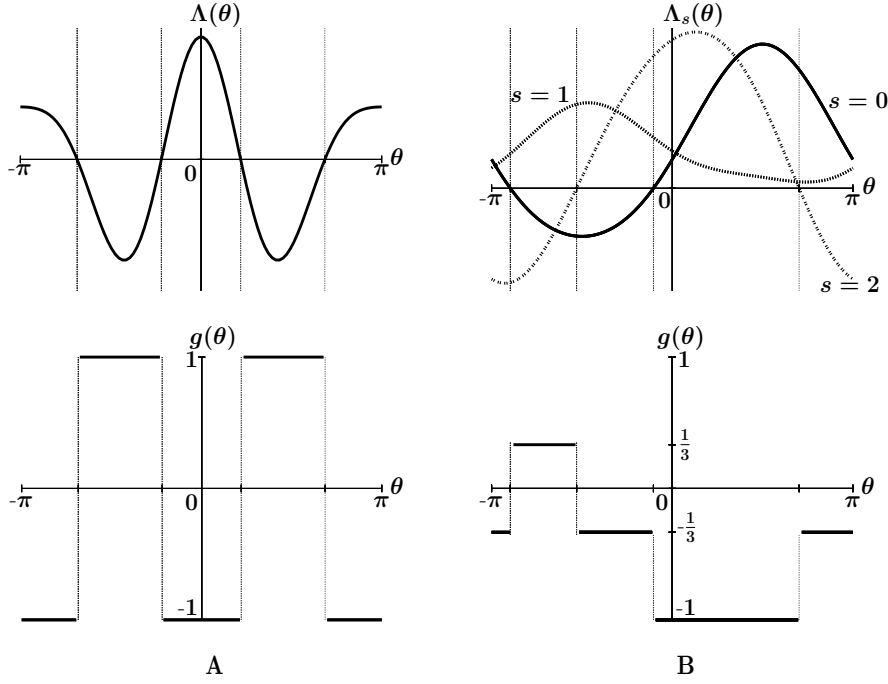


FIG. 7: The upper left plot represents the dispersion relation for a local chain, while the occupation density for its ground state is plotted below. The diagrams in the right represent respectively the bands for the dispersion relation of a local ladder with 3 rails (up) and the occupation density of its ground state (down).

First we see that the logarithmic coefficient is universal as it does not change, in general, under small changes of the couplings. It depends solely on the changes of sign in Λ . This does not apply for the constant coefficient, that changes as the zeros of Λ move.

Second, the coefficient of the logarithmic term has a simple physical interpretation: it counts the number of massless excitations in the thermodynamic limit of the Hamiltonian (zeros of Λ). This result is consistent with the conformal field theory interpretation, where the central charge in a free field theory also counts the number of massless bosons. On the other hand, if the Hamiltonian has a mass gap then Λ has constant sign and the entropy exactly vanishes. We will see how these properties can be translated to our second scenario: fermionic ladders.

Our second type of Hamiltonian corresponds to a prismatic ladder with q rails and local interactions. The Hamiltonian is

$$H = \sum_{n=1}^N \sum_{p=0}^{q-1} \sum_{j=0}^{N/(2q)} J_{p,j} a_n^\dagger a_{n+pN/q+j} + h.c., \quad (28)$$

where, as before, the couplings $J_{p,j}$ form rapidly decaying sequences in j . An example with $q = 3$ and $J_{p,j} = 0$ for $j \geq 2$, is depicted in Fig. 8.

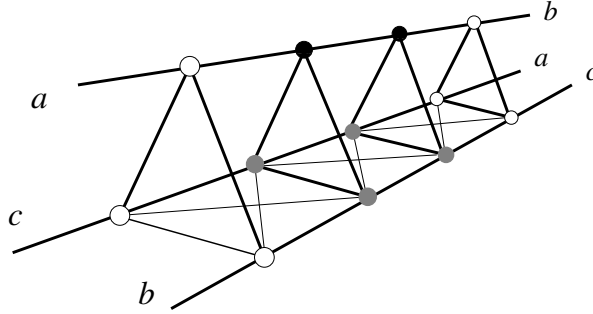


FIG. 8: Representation of a triangular ladder corresponding to the Hamiltonian of (28). The rails are joined at the end after a twist, forming therefore a twisted ring. For the sake of clarity, next to nearest neighbours interactions are represented (with thin lines) only in the lower lateral face of the ladder, but they are present in all three faces. Subsystems are represented by dark sites: the black ones represent the interval while black and grey ones represent the fragment.

The dispersion relation for this system has q bands, one for each value of the residue of $k \pmod{q}$. Namely, if $k = s \pmod{q}$ we have

$$\Lambda_k = \sum_{p=0}^{q-1} e^{2\pi i s p/q} \sum_{j=0}^{N/(2q)} J_{p,j} e^{2\pi i k j/N} + c.c.,$$

or taking the thermodynamic limit and replacing $2\pi k/N$ by the continuous variable θ we get

$$\Lambda_s(\theta) = \sum_{j=0}^{\infty} \left(\sum_{p=0}^{q-1} e^{2\pi i s p/q} J_{p,j} \right) e^{i\theta j} + c.c.$$

That is, one gets independent dispersion relations for different values of $s = 0, \dots, q-1$, we call them bands. Given the conditions for the coupling constants it is clear that every band is a smooth periodic function. A generic situation with $q = 3$ is represented in the figure 7 B. We will say that the ladder has a mass gap if the dispersion relation does not vanish at any point and we say that it is critical if some of the bands changes of sign at some angle θ_r . To every change of sign we associate a massless excitation. The example in the figure corresponds to a critical ladder with four massless particles.

From the dispersion relation one can deduce the ground state, where all the modes with negative energy (Dirac sea) are occupied. Its occupation density represents the excess of

bands with negative energy over those with positive energy at a point θ divided by q . More explicitly, we define

$$g_s(\theta) = \begin{cases} +1, & \text{if } \Lambda_s(\theta) < 0 \\ -1, & \text{if } \Lambda_s(\theta) > 0 \end{cases} \quad (29)$$

and therefore the ground state for the ladder has an occupation density given by

$$g(\theta) = \frac{1}{q} \sum_{s=0}^{q-1} g_s(\theta). \quad (30)$$

As an illustration, we plot in Fig. 7 B the occupation density corresponding to the dispersion relation represented over it. In these local ladder models, the occupation density is a piecewise constant function, like those of (16), with rational values for t_r . It is also clear that every occupation density with these characteristics can be derived from the ground states of a local ladder Hamiltonian.

Now we want to relate properties of the entanglement entropy of the ground state with those of the Hamiltonian. We will focus on two characteristics of the entropy: the existence of linear, logarithmic and constant terms and the behaviour of the coefficients under changes of the coupling constants.

One first property is that the linear term of the entropy is generically present. This is not surprising because, as it was stressed in the previous section, the correct interpretation of the *area law* in a ladder leads to a linear dependence on the size of our subsystem.

On the other hand, the logarithmic term is associated to discontinuities in $g(\theta)$ and it is zero if the theory has a mass gap and, therefore, none of the bands cross the zero value. On the contrary, the logarithmic coefficient is generically non vanishing if the theory is gapless, i.e. when some of the bands change of sign (an exception occur in the unlikely case in which two bands cross the zero value at the same point in opposite directions). The constant coefficient is in general non null when the logarithmic term is present and it is zero otherwise.

The second aspect we look at is the universality of the coefficients. The logarithmic term is always universal, it only depends on the value of the occupation density at both sides of the discontinuities and this is not affected by a small variation of the Hamiltonian. The linear term, however, is not universal in general (it depends on the position of the zeros of the dispersion relation) but it is if the theory has a mass gap. Then, $g(\theta)$ is

constant and it is not affected by small changes in the dispersion relation. Notice that in this case the logarithmic coefficient is zero.

Finally we would like to study the physical meaning of the coefficient of the logarithmic term. As discussed before, in the case of the local chain the interpretation is very simple as the term is proportional to the number of massless excitations in the theory. Here the situation is more involved because the coefficient of the logarithmic term depends not only on the number of discontinuities (massless particles) but also on the value of the occupation density at both sides of the discontinuity. Moreover, the relation between such values and the contribution to the logarithmic term is highly non trivial (20) and hard to interpret.

We believe that these difficulties have the same origin that the linear term: the choice of the subsystem X as an interval in one of the rails of the ladder (black dots in Fig. 8). Somehow, it would have been more natural to take for the subsystem an actual fragment of the ladder, i.e. equal intervals opposite to each other, one in every rail. It is represented by black and grey sites in Fig. 8. From the point of view of the chain with non-local interactions this corresponds to q intervals of size L separated by a distance $N/q - L$. The question is if one can compute the entanglement entropy of such a subsystem and if it has a simple physical meaning. The answer is yes and the result is completely compatible with the interpretation of the entropy in terms of massless particles.

Call $X_p = \{1 + pN/q, \dots, L + pN/q\}$ and consider the subsystem

$$X = \bigcup_{p=0}^{q-1} X_p$$

that actually consists of a fragment of the ladder of length L . The goal is to compute the entanglement entropy of X in the ground state with occupation density (30) in the thermodynamic limit.

To proceed, introduce for $s = 0, \dots, q-1$

$$(V_s)_{nm} = \frac{q}{N} \left(\sum_{\substack{k \in \mathcal{K} \\ k=s \pmod{q}}} e^{2\pi i k(n-m)/N} - \sum_{\substack{k \notin \mathcal{K} \\ k=s \pmod{q}}} e^{2\pi i k(n-m)/N} \right).$$

Then the matrix V in (12) is given by

$$V = \frac{1}{q} \sum_{s=0}^{q-1} V_s.$$

On the other hand one has

$$(V_s)_{n+pN/q, m+p'N/q} = e^{2\pi i s(p-p')/q} (V_s)_{nm},$$

which implies that if we introduce the matrices

$$(T_s)_{pp'} = e^{2\pi i s(p-p')/q}, \quad p, p' = 0, \dots, q-1$$

we have

$$V(X) = \frac{1}{q} \sum_{s=0}^{q-1} V_s(X_0) \otimes T_s.$$

Recall that by $V(X)$ we denote the qL -dimensional matrix obtained by restricting V to the indices that belong to X , while $X_0 = \{1, \dots, L\}$ is one of the intervals that compose X .

Now the matrices T_s commute and are diagonalised simultaneously by

$$U_{pp'} = \frac{1}{\sqrt{q}} e^{2\pi i p p' / q}$$

so that

$$(UT_s U^{-1})_{pp'} = q \delta_{s,p} \delta_{s,p'}.$$

As a result, taking all together we have

$$(I \otimes U) V(X) (I \otimes U^{-1}) = \begin{pmatrix} V_0(X_0) & 0 & \cdots & 0 \\ 0 & V_1(X_0) & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & V_{q-1}(X_0) \end{pmatrix}.$$

Where for the ground state, in the thermodynamic limit, we have

$$(V_s)_{nm} = \frac{1}{2\pi} \int_{-\pi}^{\pi} g_s(\theta) e^{i\theta(n-m)} d\theta,$$

with g_s defined in (29). Therefore if we denote by $S_{\alpha,s}(X_0)$ the Rényi entanglement entropy for the single interval X_0 in the state whose occupation density is g_s , for the entropy of the whole fragment X of the ladder, we have

$$S_\alpha(X) = \sum_{s=0}^{q-1} S_{\alpha,s}(X_0).$$

Now $S_{\alpha,s}(X_0)$ can be computed using the results of the previous section and, if ν_s represents the number of discontinuities in $g_s(\theta)$ (changes of sign in $\Lambda_s(\theta)$), we obtain

$$S_{\alpha,s}(X_0) = \frac{\alpha+1}{\alpha} \frac{\nu_s}{12} \log L + C_{\alpha,s},$$

where the constant coefficient $C_{\alpha,s}$ depends on the position of the discontinuities of $g_s(\theta)$ and not only on its number. Note that given that $g_s(\theta) = \pm 1$, the linear coefficient vanishes.

Finally the logarithmic coefficient for $S_\alpha(X)$ is

$$B_\alpha = \frac{\alpha+1}{\alpha} \frac{\sum_s \nu_s}{12}.$$

Which coincides with the conformal field theory result for a number of massless particles equal to the total changes of sign of the q bands for the dispersion relation.

VIII. CONCLUSIONS AND FINAL COMMENTS

In this paper we have studied the Rényi entanglement entropy for a subsystem of a unidimensional fermionic chain in a general, translational invariant state that can be described by a Slater determinant.

Although the computational time, in principle, grows exponentially with the size of the subsystem we can circumvent this limitation and go to large sizes by employing the relationship between the reduced density matrix of the subsystem and the corresponding correlation matrix. In this way, we can compute easily the Rényi entropy through the spectrum of the correlation matrix restricted to the chosen subsystem. It is important to highlight that this method is only valid when the chain is in an state which fulfils the Wick decomposition property. Inside this set of states, there is a kind of configurations (i.e. the factorised momentum states) in which the total correlation matrix is Toeplitz. In this case, if the subsystem is a single interval of contiguous sites in the coordinate space its correlation matrix is Toeplitz as well.

Taking the thermodynamic limit and periodic boundary conditions we have found the behaviour of the Rényi entropy with the length of the interval, using the Fisher-Hartwig conjecture for Toeplitz determinants. We have computed the different coefficients for the expansion of the entropy and we present explicit, general expressions for the logarithmic

and constant terms, that were not known in the literature. In order to do so we apply a new strategy that allows to circumvent the problem of the presence of divergences that finally cancel out. A simple integration by parts in the complex integral shows the automatic cancellation of divergences, renders the integrals finite and makes the computations much simpler. As remarked before, neither the technical tool for the cancellation of divergences nor the explicit expression for the coefficients were previously known.

We have also checked numerically the validity of this expansion for three particular states. The first of them corresponds to the ground state of a local Hamiltonian, in which case we can compare our results with those derived from conformal field theory. We have shown the perfect agreement between both approaches. The other two states can be viewed as the lowest energy state of non-local Hamiltonians, which is illustrated with two simple examples.

Finally, we discuss the physical insights that we can get from the previous expansions. In order to do that we study the ground state of Hamiltonians corresponding to local chains and ladders for which the results of section V apply. We analyse the universality of the coefficients and compare our results with those derived from general arguments in conformal field theory. In particular we show that in the case of fermionic ladders the latter considerations can also be applied if we take a fragment, instead of an interval, for our subsystem.

A natural extension of our work is the study of the entropy for a subsystem composed of several disjoint intervals. There are some recent works where this problem is addressed for the ground state of a local chain [21–24]. We would like to consider a general energy eigenstate like those in the present paper.

A first step in this direction, that we took in section VII, is the computation of the entanglement entropy for the fragment of the ladder. This can be seen, actually, as a collection of disjoint intervals, but in very particular positions so that the techniques for Toeplitz determinants and the Fisher-Hartwig conjecture can still be applied.

In the general case however, for intervals in generic positions, the reduced density matrix of the subsystem is not Toeplitz any more, so we can not use the Fisher-Hartwig conjecture and the present results do not apply. The study of the expansion of the entanglement entropy for such a subsystem will be the subject of further research.

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